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DETAILED MODELLING OF COMBUSTION: A NON-INTERFERING DIAGNOSTIC --ETC(U)
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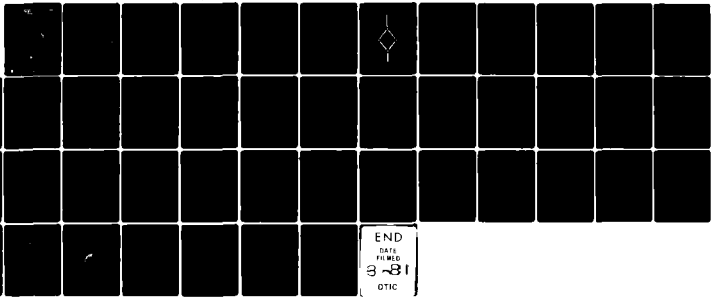

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Detailed Modelling of Combustion: A Non-Interfering Diagnostic Tool

E. S. Oran, J. P. Boris, and M. J. Fritts

Laboratory for Computational Physics

January 19, 1981

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A major goal of detailed numerical modelling of combustion is to develop computational tools which can be used interactively with laboratory diagnostic techniques to interpret and understand experiments. Only through this quantitative interaction of prediction and measurement can we calibrate convincingly our understanding of the fundamental physical and chemical processes involved. Modelling of flames and detonations is particularly challenging because of the strong feedback between the energy released due to chemical reactions and the evolution of the hydrodynamic flow. Since it is generally not possible to decouple these processes completely, special numerical techniques are required to solve the problems. In this paper, the basic steps and decisions which must be

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20. Abstract (Continued)

made when constructing and using a numerical model will be disucssed. These involve 1) choosing the numerical algorithms based on the physics and chemistry of the problem. 2) testing the model based on these algorithms in different limits against theoretical and analytical results, and 3) using the model interactively with experiments. With the third step specifically in mind, it will be shown how the species concentration, velocity, and temperature profiles obtained from laser probe diagnostics can provide information for use in and comparison with detailed calculations.

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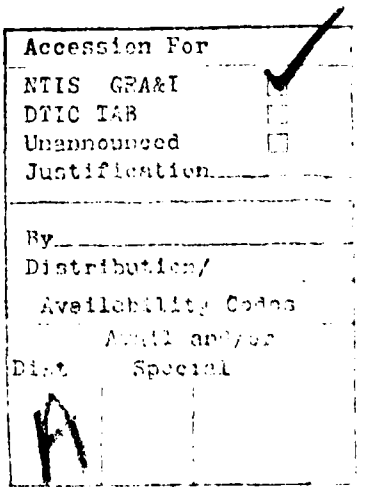


DETAILED MODELLING OF COMBUSTION: A NON-INTERFERING DIAGNOSTIC TOOL

I. Introduction

Detailed modelling, or numerical simulation, provides a method we can use to study complex reactive flow systems.[1] Using this technique, predictions about the behavior of a physical system are obtained by solving numerically the multi-fluid conservation equations for mass, momentum, and energy. Since the success of detailed modelling is coupled to the ability to handle an abundance of theoretical and numerical detail, this field has matured in parallel with the increase in size and speed of computers and sophistication of numerical techniques.

It is important to distinguish between empirical, phenomenological and detailed models. Empirical models are constructed from data obtained by experiments, summarized in analytical or numerical form, and subsequently tested against proven theoretical laws or other data. Phenomenological models are extrapolations from theory based on our physical intuition which must be tested against experimental data. The shortcomings of the empirical models lie in their limited range of validity, while phenomenological models become more tenuous as they approach the complexities of real physical systems.

Detailed models usually contain parts which may be empirical or phenomenological in origin. However, detailed modelling attempts to overcome these shortcomings by incorporating theoretical detail rich enough to approximate reality; detail far richer than could be summarized in any succinct analytical model, yet more theoretically sound than standard phenomenological models or empirical fits.

Manuscript submitted November 6, 1980.

The purpose of this paper is to present an overview and an assessment of the current state of detailed modelling as applied to combustion systems. We will attempt to familiarize the reader with the goals, terminology and inherent problems in modelling combustion systems. The emphasis is not on presenting a full set of complicated multi-fluid equations or on explaining the numerical algorithms required to solve the governing equations. Instead we hope to impart a sense of the power and role of detailed modelling, an understanding of why physical insight must be built into numerical algorithms, and an indication of how to test these models at every stage of construction against both theory and experiment.

Figure 1 depicts the role of both analytical and numerical modelling with respect to experiments. Increased accuracy and reliability are required in proceeding from the evaluation of concepts to engineering design. The "calibration" of our understanding has been given the pivotal central location. From experimental observation and approximate theoretical models we can postulate quantitative physical laws which we expect an effect to obey. These "laws" can be tested against reality by incorporating them in a detailed model which makes quantitative predictions for series of experimental measurements.

A computer simulation using a detailed model is similar to an experiment in that it will not give simple functional forms among physical variables. Each calculation is like a unique experiment performed with one set from an infinity of possible sets of geometric, boundary, and initial conditions. Just as valid results can be

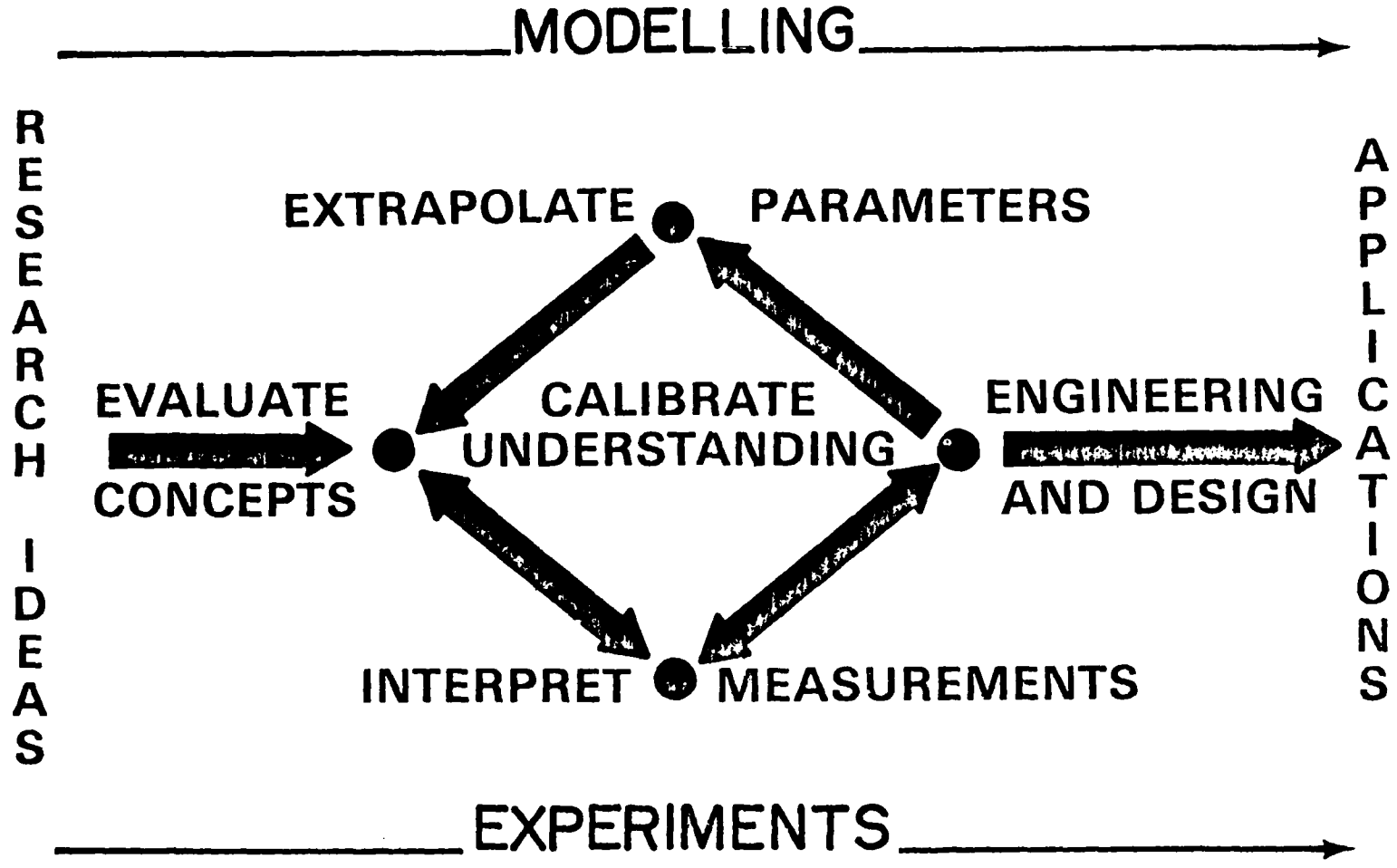


Fig. 1 - Schematic diagram showing how modelling and experiments can be used interactively to increase our understanding of complicated systems and to use this understanding to help in practical designs.

extracted from an experiment only through an understanding of the effects and limitations of the instruments used in collecting the data, results obtained using detailed modelling must be examined in the light of the limitations inherent in its tools, both analytical and numerical. The first section of this paper will therefore deal with an exposition of the problems inherent in detailed modelling of combustion systems so that as we proceed we have a healthy respect both for the magnitude of the problems and the limitations of our methods.

The next section will concentrate on the choice of numerical algorithms used in the models. This process corresponds to the construction and design of experimental apparatus which must reflect a good knowledge of the physics the experiment is to study. Modelling combustion systems has its own particular problems because of the strong interaction between the energy released from chemical reactions and the dynamics of the fluid motion. Release of chemical energy generates gradients in temperature, pressure, and density. These gradients, in turn, influence the transport of mass, momentum, and energy in the system. On a large scale, the gradients may generate vorticity or effect the diffusion of mass and energy. On a more microscopic scale, they are the origin of the turbulence which drastically affects macroscopic mixing and burning velocities. In modelling shocks, detonations, or flame propagation, time and space scales of interest can span as many as ten orders of magnitude. Thus to obtain adequate resolution, the numerical methods must be computationally fast as well as accurate. Methods must be developed which rely on asymptotic solution techniques to follow short time and space scale phenomena on a macroscale. It is in this aspect

that detailed modelling most closely approximates experiment. If our numerical apparatus cannot resolve the basic controlling physical processes, no meaningful calculations can be made of their effects.

Although detailed modelling does not directly provide the types of useful analytic relationships which guide our intuition and allow us to make quick estimates, it gives us the flexibility to evaluate the importance of a physical effect by simply turning it off or on or changing its strength. The model can also be used to test the sensitivity of the physical results to independent theoretical approximations. Those analytic results which are available are valuable in benchmarking the model in various limits. A series of tests which compare analytic results to numerical simulations may calibrate the simulation before it is compared to experiments or used for extrapolation. Conversely, a well-tested detailed model serves as a very useful means of calibrating unknown parameters and form factors in approximate theories.

The last two sections of this paper will discuss this interplay between detailed modelling and theory and experiment. The third section describes how a model must be tested in various limits for physical consistency to insure its accuracy. The specific example chosen here is a comparison between an analytic solution and a detailed numerical simulation of a premixed laminar flame. The last section shows how a comparison between models results and experiments can be used to calibrate the model and to guide further experiments. The example chosen is a calculation of flow over an immersed object which is compared to both experimental and theoretical results.

II. Problems in Modelling Reactive Flows

Errors and confusion in modelling arise because the complex set of coupled, nonlinear, partial differential equations are not usually an exact representation of the physical system. As examples, first consider the input parameters, such as chemical rates or diffusion coefficients. These input quantities, used as submodels in the detailed model, must be derived from more fundamental theories, models or experiments. They are usually not known to any appreciable accuracy and often their values are simply guesses. Or consider the geometry used in a calculation. It is often one or two dimensions less than needed to completely describe the real system. Multidimensional effects which may be important are either crudely approximated or ignored. This lack of exact correspondence between the model adopted and the actual physical system constitutes the basic problem of detailed modelling. This problem, which must be overcome in order to accurately model transient combustion systems, can be analyzed in terms of the

- multiple time scales,
- multiple space scales,
- geometric complexity, and/or
- physical complexity

of the systems to be modelled.

The first class of problems arises as the result of trying to represent phenomena characterized by very different time scales. In ordinary flame and detonation problems these scales range over many orders of magnitude. When phenomena are modelled that have characteristic times of variation shorter than the timestep one can afford, these

phenomena are usually called "stiff." Sound waves are stiff with respect to the timestep one wishes to employ when modelling a subsonic flame speed. Many chemical reaction rates are stiff with respect to convection, diffusion, or even sound wave timestep criteria. Two rather distinct modelling approaches, global implicit and timestep-split asymptotic, have been developed to treat these temporally stiff phenomena. These two approaches are briefly described later in this paper.

The second class of problems involves the huge disparity in space scales occurring in combustion problems. To model the steep gradients at a flame front, a cell spacing of 10^{-3} cm or smaller might be required. To model convection, grid spacings of 1 to 10 cm might be adequate. Complex phenomena such as turbulence which occur on intermediate spatial scales present a particular modelling problem. It would be a pipedream to expect a numerical calculation to faithfully reproduce physical phenomena with scale lengths shorter than a cell size. Therefore, to calculate realistic profiles of physical variables, a certain cell spacing is required to obtain a given accuracy. Choosing a method which maximizes accuracy with a minimum number of grid points is a major concern in detailed modelling.

The third set of obstacles arises because of the geometric complexity associated with real systems. Most of the detailed models developed to date have been one-dimensional, but this gives a very limited picture of how the energy release affects the hydrodynamics. Even though many processes in a combustion system can be modelled in

one-dimension, there are others, such as boundary layer growth, or the formation of vortices and separating flows, which clearly require at least two-dimensional hydrodynamics. Real combustion systems are at least two-dimensional, with unusual boundary conditions and internal sources and sinks. However, even with sixth generation parallel processing computers available, what can be achieved with two-dimensional detailed models is still limited by computer time and storage requirements.

In the current state-of-the-art, one-dimensional models can best be used to look in detail at the coupling of a very large number of species interactions in a geometry that is an approximation to reality. Processes such as radiation transport, turbulence, or the effects of heterogeneity of materials can be included either as empirically or theoretically derived submodels. Two- and three-dimensional models are best used to study either gross flow properties or detailed radiation transport. In these latter models, the chemical reaction scheme is usually quite idealized or parameterized.

The final set of obstacles to detailed modelling concerns physical complexity. Combustion systems usually have many interacting species. This leads to sets of many coupled equations which must be solved simultaneously. Complicated ordinary differential equations describing the chemical reactions or large matrices describing the molecular diffusion process are costly and increase calculation time orders of magnitude over idealized or empirical models. Table 1 lists some of the major chemical and physical processes which have to be considered for

an accurate description of a complicated combustion system. Multi-phase processes such as surface catalysis and soot formation can be important even when we are primarily interested in gas phase combustion. For most interesting systems, one finds that the basic chemical reaction scheme, the individual chemical rates, the optical opacities, or the effects of surface reactions are not well known. Before a model of a whole combustion system can be assembled, each individual process must be separately understood and modelled. These submodels are either incorporated into the larger detailed model directly or, if the time and space scales are too disparate, they must be fit in phenomenologically. For example, diffusion and thermal conductivity between a wall and the reacting gas can be studied separately and then incorporated directly into a detailed combustion model. Turbulence, however, can be modelled on its own space scales only in idealized cases. These more fundamental models must be used to develop phenomenological models for use in the macroscopic detailed model. Resolution and computational cost prevent incorporating the detailed turbulence model directly.

Table 1
Fundamental Processes in Combustion

	gas phase	multi-phase
Chemical kinetics	↓	↓
Hydrodynamics-laminar	↓	↓
Thermal conductivity, viscosity	↓	↓
Molecular diffusion	↓	↓
Thermochemistry	↓	↓
Hydrodynamics-turbulent	↓	↓
Radiation	↓	↓
Nucleation	⋮	↓
Surface Effects	⋮	↓
Phase Transitions (Evaporation, condensation...)	⋮	↓

Often there are cases where the submodels are poorly known or misunderstood, and this may cause the modellers no end of grief. A typical example is shown in Fig. 2 which was provided by David Garvin at the U. S. National Bureau of Standards. The figure shows the rate at 300°K for the reaction $HO + O_3 \rightarrow HO + O_2$ as a function of the year of the measurement. We note with amusement and chagrin that if we were modelling a kinetics scheme which incorporated this reaction before 1970, the rate would be uncertain by five orders of magnitude! Similar tales of horror also exist for thermochemical data. In combustion and atmospheric physics, detailed models have been used to bound and test the importance of chemical rates. Some of these combustion applications will be described below.

In order to illustrate how the problems caused by the requirements of temporal and spatial resolution and geometric and physical complexity are translated into computational time, we have chosen to analyze a gedanken flame experiment. Consider a closed tube one meter long which contains a combustible gas mixture. We wish to calculate how the physical properties such as temperature, species densities, and position of the flame front change after the mixture is ignited at one end. The burning gas can be described, we assume, by a chemical kinetics reaction rate scheme which involves some tens of species and hundreds of chemical rates, some of which are "stiff". We will assume one-dimensional propagation along the tube. Boundary layer formation and turbulence will be ignored. We further assume that the flame front moves at an average velocity of 100 cm/sec.

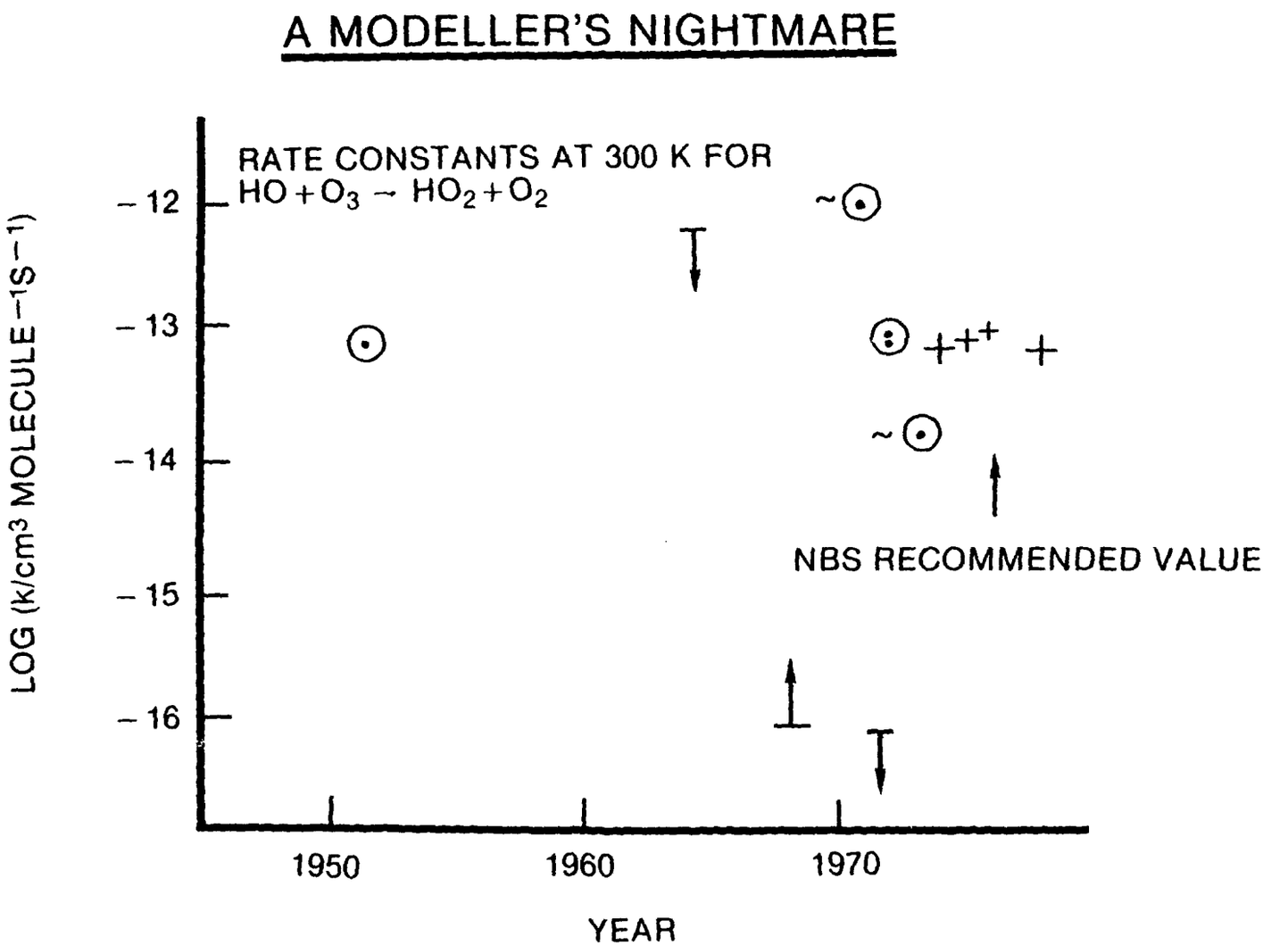


Fig. 2 - Measured values of the rate constant for $HO + O_3 \rightarrow HO_2 + O_2$ as a function of the year of measurement. The arrows with overbars and underbars indicate measured upper and lower bounds, respectively. (Courtesy of David Garvin, U. S. National Bureau of Standards).

Table II summarizes the pertinent time and space scales in this problem. Assuming the speed of sound is 10^5 cm/sec, a timestep of about 10^{-9} sec sould be required to resolve the motion of sound waves bouncing across the chamber. Chemical timescales, as mentioned above, are about 10^{-6} sec. This number may be reduced drastically if the reaction rates or density changes are very fast. It takes a sound wave about 10^{-3} seconds to cross the 1 meter system and it takes the flame front about one second to cross. We further assume that the flame zone is about 10^{-2} cm wide and that it takes grid spacings of 10^{-3} cm to resolve the steep gradients in density and temperature, In those portions of the tube on either side of the flame front, we assume that 1 cm spacings are adequate.

Table II
Important Scales in Gedanken Flame Calculation

Timescales		Spacescales	
Δt	sec	Δx	cm
Sound Speed	10^{-9}	Flame Resolution	10^{-3}
Chemistry	10^{-6}	Flame Zone	10^{-2}
Sound Transit Time	10^{-3}	Diffusion Scale	10^{-1}
Flame Transit Time	1	Convective Scales	10
		System Size	100
	$V_f = 100$	cm/sec	

To estimate the computational expense of this calculation, we use 10^{-3} seconds of computer time as a reasonable estimate of the time it takes to integrate each grid point for one timestep (a single point-step). This estimate includes a solution of all of the chemical and hydrodynamic equations and is based on a detailed model of a hydrogen-oxygen flame problem optimized for a parallel processing computer.

Figure 3 shows the information in Table II cast into a graph of space versus time. Since the scales are logarithmic, a calculation of the number of point-steps and then of the needed computer time requires exponentiation. Thus it appears that 3000 years of computer time is required to calculate the 10^{14} point-steps involved in representing the finest resolved space and time scales!

Of course this is unacceptable. Ideally such a simple calculation should take about 100 seconds. What are needed are numerical algorithms which have the resolution in time and space only where it is required. Furthermore, these algorithms should be optimized to take advantage of what is known about the physics and chemistry of the problem. This will be discussed further below where it is shown how the application of various numerical algorithms can be used to reduce this flame system to a tractable computational problem.

Turbulence is one of the outstanding problems of reactive flow modelling and is another excellent example of the difficulty we have in resolving highly disparate time and space scales. Our understanding and eventual ability to predict the complicated interactions occurring in turbulent reactive flow problems is imperative for many combustion modelling applications. The presence of turbulence alters mixing and reaction times and heat and mass transfer rates which in turn modify the local and global dynamic properties of the system. What we need to resolve these problems are accurate yet compact phenomenological turbulence models which can be used to describe realistic combustor systems, open flames, and other turbulent reactive flows confidently

DIRECT SOLUTIONS WITH SOUND WAVES AND A UNIFORM GRID

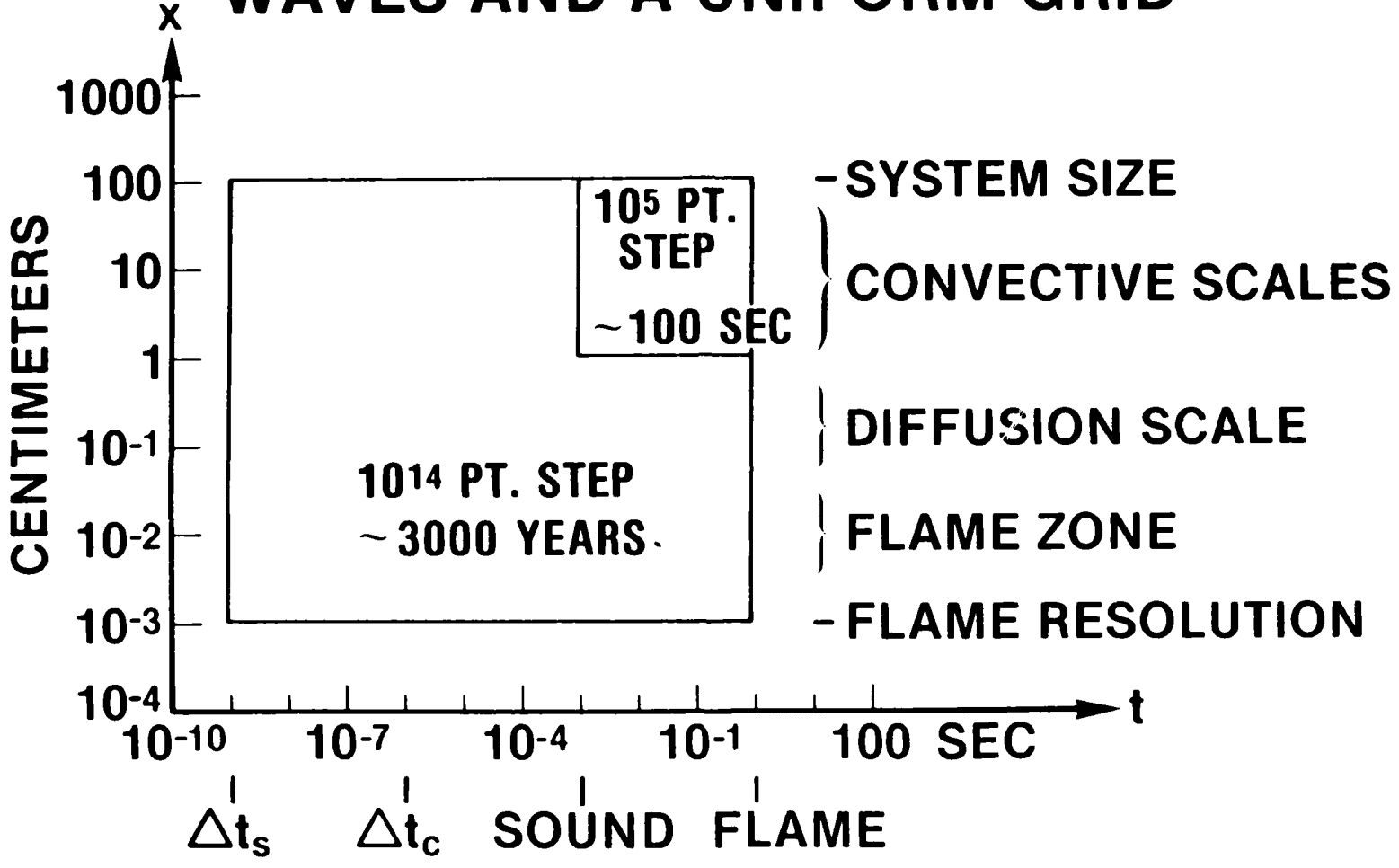


Fig. 3 - Space and time scales in the gedanken flame calculation. A naive direct solution of the problem could take 3000 years of computer time. The calculation should be possible in 100 seconds.

and efficiently. These computational models must decouple the subgrid turbulence and microscopic instability mechanisms from calculations of the macroscopic flow. Below we list the important properties of an ideal turbulence model [2].

1. Chemistry-Hydrodynamic Coupling and Feedback

Explicit energy feedback mechanisms from mixing and reactions to the turbulent velocity field and the macroscopic flow must be formulated. The "laminar" macroscopic flow equations contain phenomenological terms which represent averages over the macroscopic dynamics to include the effects of turbulence. Examples of these terms are eddy viscosity and diffusivity coefficients and average chemical heat release terms which appear as sources in the macroscopic flow equations. Besides providing these phenomenological terms, the turbulence model must use the information provided by the large scale flow dynamics self-consistently to determine the energy which drives the turbulence. The model must be able to follow reactive interfaces in the macroscopic scale.

2. Modelling Onset and other Transient Turbulence Phenomena

The model should be able to predict the onset of turbulence in initially laminar flow since bursts and other highly transient phenomena seem to be the rule in reactive flow turbulence. Gradients in density, temperature, and velocity fields in the reacting fluid drive the macroscopic fluid dynamic instabilities which initiate turbulence. Thus these gradients from the macroscopic calculation are bound to be key ingredients in determining the energy available to drive the turbulence.

3. Complicated Reactions and Flow

The ideal turbulence model must deal with multiscale effects within the subgrid model. If there is a delay as velocity cascades to the short wavelength end of the spectrum due to chemical kinetics or buoyancy, for example, the model must be capable of representing this. Otherwise bursts and intermittency phenomena cannot be calculated.

4. Lagrangian Framework

An ideal subgrid model should be constructed on a Lagrangian hydrodynamics framework moving with the macroscopic flow. This requirement reduces purely numerical diffusion to zero so that realistic turbulence and molecular mixing phenomena will not be masked by non-physical numerical smoothing. This requirement also removes the possibility of masking purely local fluctuations by truncation errors from the numerical representation of macroscopic convective derivatives. The time-dependent (hyperbolic) Lagrangian framework should also generalize to three dimensions as well as resolve reactive interfaces dynamically.

5. Scaling

Breaking a calculation into macroscopic scales and subgrid-scales is an artifice to allow us to model turbulence. The important physics occurs continuously over the whole spectrum from k_o, the wavenumber corresponding to the system size, to $k_{diss.}$, the wave number corresponding to a mean free path of a molecule. Thus the macroscopic and subgrid scale spectra of any physical quantity must couple smoothly at k_{cell}, the cell boundary wave number. If this number were to be changed, as might happen if numerical resolution were halved or doubled, the predictions of the turbulence model must not change.

6. Efficiency

Of course, the model must be efficient. The number of degrees of freedom required to specify the status of turbulence in each separately resolved subgrid region has to be kept to a minimum for the model to be generally useable. The real fluid has essentially an infinite number of degrees of freedom to represent the state of the gas in each small element. We would like to be able to do the job with a minimal number of degrees of freedom.

III. Choosing an Algorithm Based on the Physics of the Problem

In reactive flow calculations we are concerned with two flow regimes which depend on the rate of energy release. When energy is released quickly, shocks and detonations are formed. When energy is released slowly, flames are formed. The former requires that the numerical algorithm used follow the changes of the system on timescales determined by the speed of sound in the material (Courant condition). If we follow this same timescale in the flame case, in which the physical timescales of interest are much larger, the cost is exhorbitant. The gedanken flame calculation described above cost so much partly because we postulated the use of an explicit algorithm based on timesteps determined by the Courant condition. For flame calculations, then, the answer is to use techniques in which the energy conservation equation is converted to a pressure equation which is solved implicitly.

The problem is basically that of coupling into one calculation all

of the pertinent physical and chemical processes characteristic of a combustion system. Two distinct approaches have evolved. In the first of these, often called "global implicit" differencing, the complete set of nonlinear coupled equations describing the physical system of interest is cast into a simple finite-difference form. The spatial and temporal derivatives are discretized and the nonlinear terms are linearized locally about the solutions obtained numerically at the previous timestep. This process is valid only when the values of the physical variables change slowly over a timestep. A rigorously correct treatment of the nonlinear terms requires iteration and large matrices must be inverted at each timestep to guarantee stability. In one spatial dimension the problem usually appears as a block tridiagonal matrix with M independent physical variables to be specified at N_x grid points. Then an MN_x by MN_x matrix must be inverted at each iteration of each timestep. The blocks on or adjacent to the matrix diagonal are M x M in size so the overall matrix is quite sparse. Nevertheless, an enormous amount of computational work goes into advancing the solution even a single timestep. Multidimensional problems, in this approach, lead to matrices which are MN_xN_y by MN_xN_y in two dimensions and $MN_xN_yN_z$ by $MN_xN_yN_z$ in three dimensions. In complex kinetics problems with no spatial variation, the M independent variables are the species number densities and temperature in the homogeneous volume of interest. The Gear method [3] is an example of this global implicit approach for pure kinetics problems.

The second approach is a fractional-step method we call asymptotic timestep-splitting. It is developed by consideration of the

specific physics of the problem being solved. Stiffness in the governing equations is usually handled "asymptotically" rather than implicitly. The individual terms, including those which lead to the stiff behavior, are solved as independently and accurately as possible. Examples of such methods include the Selected Asymptotic Integration Method [4,5] for kinetics problems and the asymptotic slow flow algorithm for hydrodynamic problems where the sound speed is so fast that the pressure is essentially constant [6,7].

The tradeoffs between these two approaches are clear. The implicit approach puts maximum strain on the computer and minimal strain on the modeller. For this method, convergence of the computed solutions is easy to test with improved temporal and spatial resolution. Non-convergence of any particular calculation may be hard to spot since severe numerical damping has been introduced to maintain numerical stability and positivity. This damping changes the desired profiles quantitatively, although quickly detected qualitative errors are often smoothed out. Solutions may be wrong yet stable.

In contrast, the asymptotic approach puts minimal strain on the computer but demands much more of the modeller. The convergence of the computed solutions is usually easy to test with respect to spatial and temporal resolution, but situations do exist where, for example, reducing the timestep can make an asymptotic treatment of a "stiff" phenomenon less accurate rather than more accurate. This follows because the disparity of timescales between fast and slow phenomena is often exploited in the asymptotic approach rather than tolerated.

Furthermore, the non-convergence of any particular solution is often easier to spot in the asymptotic approach because the manner of degradation is usually catastrophic. In kinetics calculations, lack of conservation of mass or atoms signals inaccuracy rather clearly.

The asymptotic approach usually leads to more modular simulation models than the global implicit approach. Hydrodynamics, transport, equation of state calculations, and chemical kinetics are tied neatly into individual packages. What is even more important, specialized techniques for enhancing accuracy can be incorporated at each stage and for each physical phenomenon being modelled separately. There is no need to use simpler methods which are suitable for inclusion into a single giant finite difference formula. Since each phenomenon is treated as an independent package, the full spectrum of numerical tricks is applicable.

These packages are relatively easy to test individually and can be very sophisticated. They can also be used directly in a number of totally different physical problems with little or no change and are hence more flexible than equivalent portions of a global implicit algorithm. The price for this flexibility is the need to treat carefully all the couplings between the individual physical terms and effects. Using the asymptotic approach one cannot sit back and turn a massive mathematical crank to get an answer.

At this point the pros and cons of the two approaches seem to roughly counterbalance; they have been presented that way purposely. This apparent equity extends to most accuracy criteria as well. If

an interesting timescale is not resolved, neither solution method can give detailed profiles of phenomena occurring on that scale. Similarily, to compute spatial gradients accurately they must be resolved with enough spatial grid points in either type of calculation.

The fact that the asymptotic approach demands more work of the physicist is counterbalanced by the work that must be done to reduce the computational expense of using the global implicit method. This calculational expense, above all else, is the factor which has caused us to employ asymptotic rather than global implicit formulations. For example, solving a chemical kinetics scheme for M species requires inverting a general matrix of size $M \times M$. This involves approximately M^3 operations. In contrast, the selected asymptotic approach to solving the kinetics equations generally scales as M. It is one goal of detailed modelling to be able to include the full details of extremely complex kinetics systems coupled to time-dependent fluid dynamics. Since more complex problems can be solved for the same cost using asymptotics, we are willing to invest the effort in the physics modules and their coupling in order to be able to expand our computational abilities.

Using the information discussed so far, we can now return to the gedanken flame calculation with the idea of modifying our numerical methods in order to reduce the computational cost. The goal is to calculate the propagation of a flame front across a one-meter tube using a one-dimensional geometry and given a fixed detailed chemical reaction rate scheme.

First, we recognize immediately that we are interested in calculating a flame front moving at less than the local sound speed. Thus either a slow flow approximation or any method which treats pressure implicitly would eliminate the sound speed criterion on the timestep. By using the asymptotic slow flow technique described below and still assuming a uniform grid spacing, the number of point-steps is reduced from 10^{14} to 10^{11}. Thus Fig. 4 shows that the time required for the calculation is reduced from 3000 to 3 years!

But this is still atrocious, and we must now face the problem of eliminating unnecessary grid points. Adaptive gridding is currently a frontier in reactive flow modelling. As we have mentioned above, there are no excellent techniques. The block on the graph in Fig. 5 shows the region spanned in the gedanken flame problem by an adaptively gridded calculation. Here 100 cells of 1 cm length are used and the region surrounding the flame front is finely gridded with 100 additional cells of 10^{-3} cm length. The timestep is still governed by the smallest cells, but by now only 200 cells are needed rather than 10^5. The saving, about a factor of 500, reduces the computational time to 2×10^8 point-steps, or about two days.

Finally, Fig. 6 summarizes the computational expense of performing the flame propagation problem using the possible, but as yet unexploited, technique of adaptive intermittent gridding. The idea here is that a finely gridded region is injected into the calculation at intermittent timesteps. This is done often enough to update the properties of the finely-spaced region which are then used as interior boundary conditions for the coarsely-spaced region. Now assume that 100 cells are needed to resolve the flame zone. Further, 100 short timesteps are

DIRECT SOLUTIONS WITH SLOW FLOW, ASYMPTOTICS, AND UNIFORM GRID

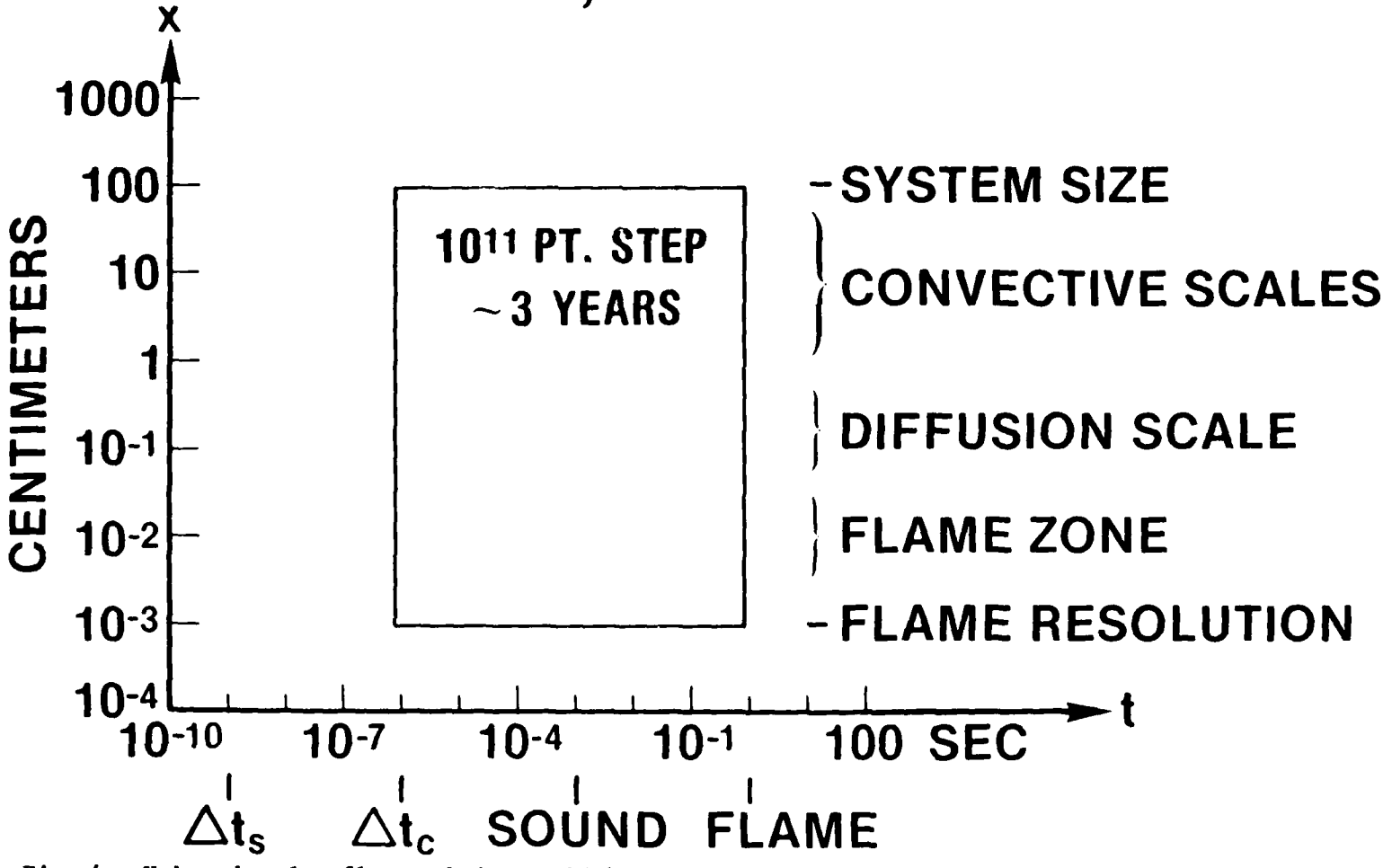


Fig. 4 - Using the slow flow technique, which allows us to follow timescales larger than those required by an explicit solution of the energy equation, reduces the required computational time to three years.

ADAPTIVE GRIDDING WITH SLOW FLOW AND ASYMPTOTIC CHEMISTRY

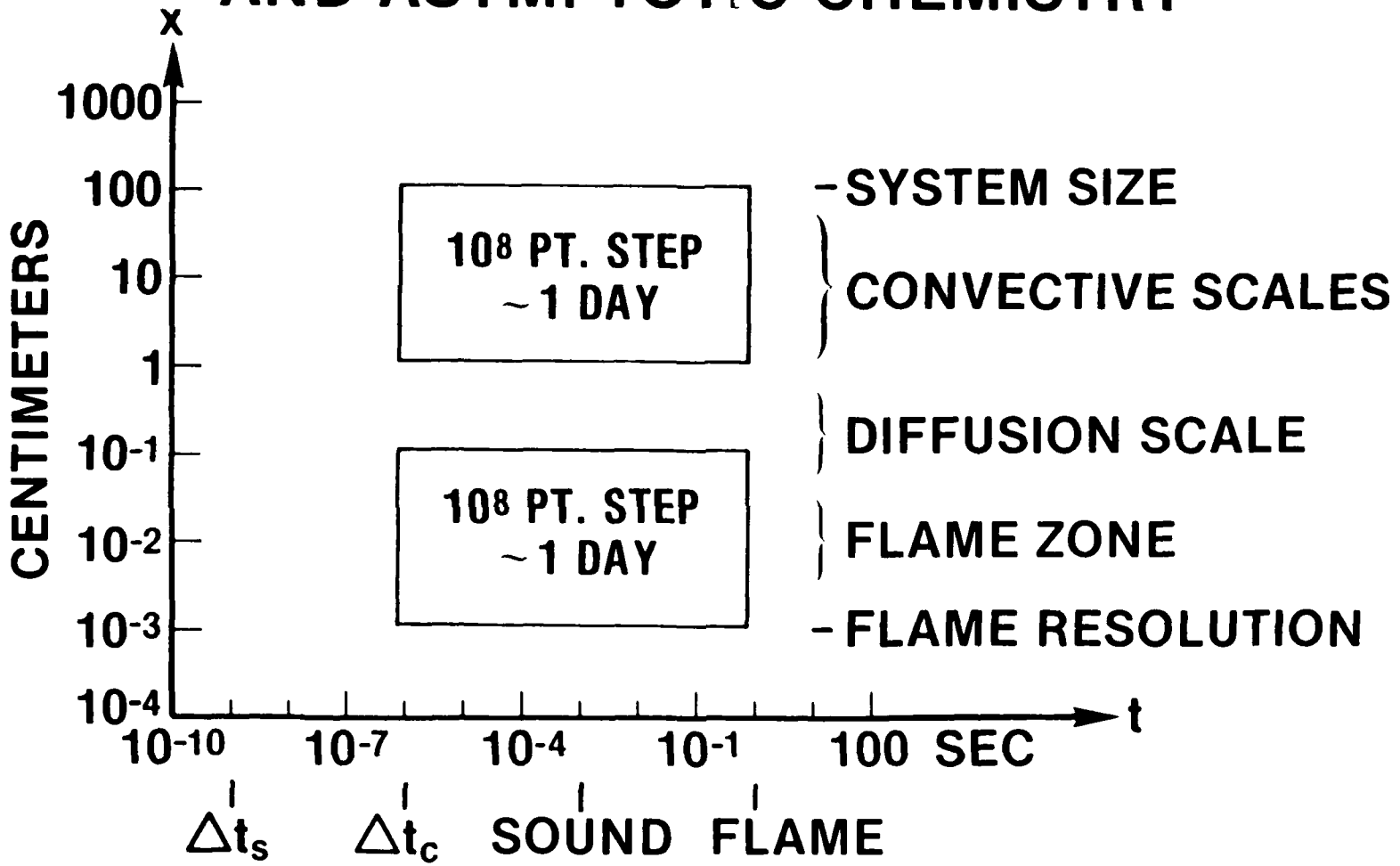


Fig. 5 - An adaptive gridding method, in which the fine resolution is clustered around the flame front, reduces computational time to two days

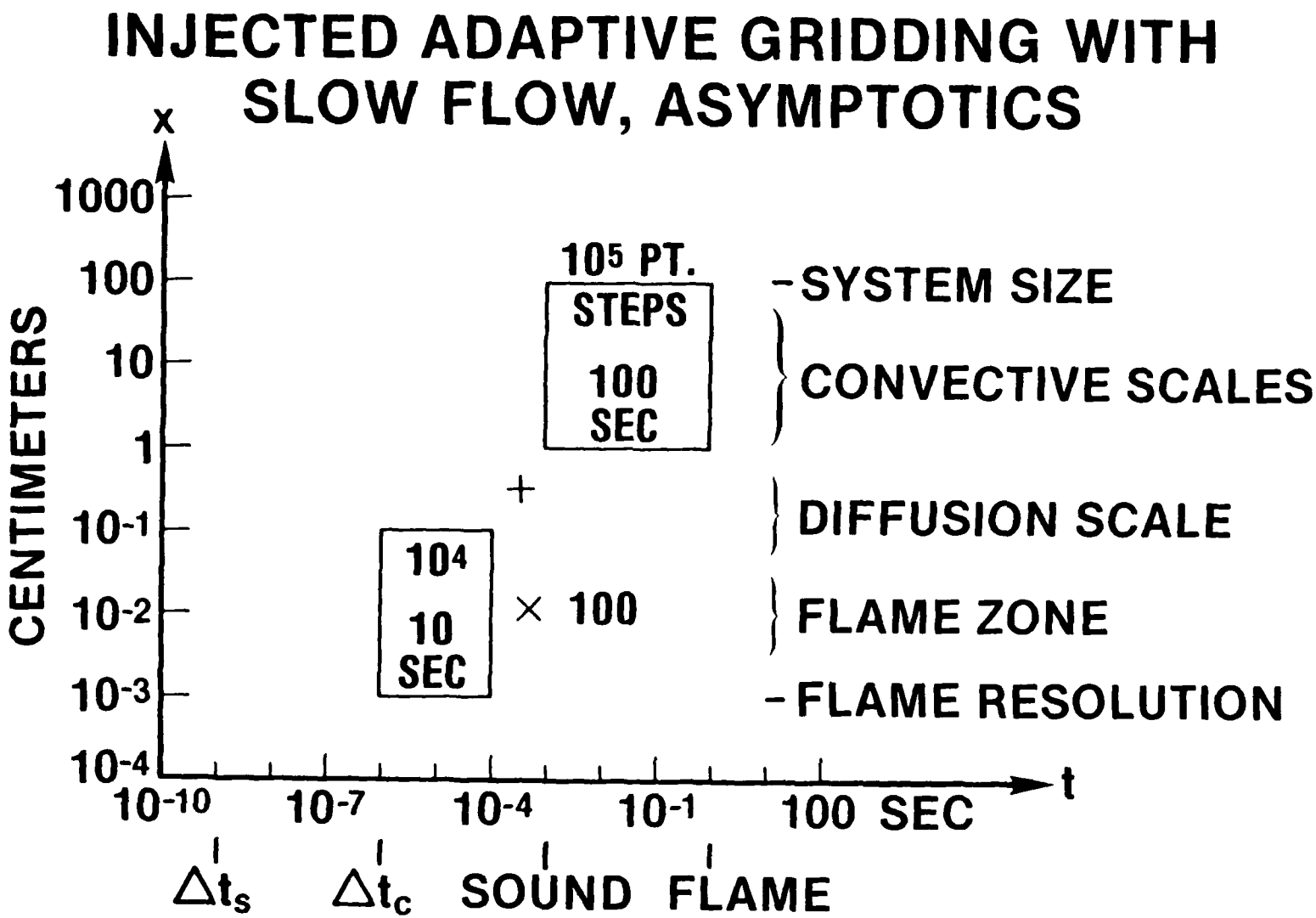


Fig. 6 - The as yet undeveloped injected adaptive gridding method will reduce the computational time to 1100 seconds

enough to resolve changes in the flame zone brought about by the relatively slowly changing outer boundary conditions. During the imbedded calculation, the flame front moves only 10 of the fine zones, which is sufficient to determine flame speed and boundary conditions to be used in the coarsely spaced calculation. The imbedded calculation may be done once in each large cell. Thus a total of 100 + (100)(10) = 1100 seconds of computational time is required for the large scale simulation.

This example has illustrated the importance of using the appropriate algorithm motivated by considerations of the actual problem that must be resolved. It has further illustrated how much may be accomplished by developing the methods of adaptive gridding. One point that has not been mentioned, however, is that much of the cost of a detailed reactive flow calculation is taken up by the integration of the ordinary differential equations describing the chemical kinetics. Using the latest asymptotic techniques improves the picture painted above by a factor of two to four. But further improvements in the integration time of ODE's without sacrificing accuracy is certainly an area where development is needed.

IV. Testing the Model Against Theoretical Results

Analytical solutions, while often approximate, are extremely useful in providing functional relationships and generalizing trends. Below we show that by comparing numerical and analytic results, we can gain new insights into the controlling physical processes.

Ignition of a fuel-oxidizer mixture occurs when an external source

of energy initiates interactions among the controlling convective, transport and chemical processes. Whether the process results in deflagration, detonation, or is simply quenched depends on the intensity, duration, and volume affected by an external heat source. Ignition also will depend on the initial ambient properties of the mixture which determine the chemical induction time and the heat release per gram. Thus ignition is a complicated phenomena and its prediction for a specific mixture of homogeneous, premixed gases depends strongly on input parameters which are often very poorly known. A convenient, inexpensive way to estimate whether a mixture will ignite given a heat source intensity, duration, and volume would be a valuable laboratory tool and a useful learning device.

A closed form similarity solution for the nonlinear time-dependent slow-flow equations has been used as the basis for a simple, time-dependent, analytic model of localized ignition which requires minimal chemical and physical input [8]. As a fundamental part of the model, there are two constants which must be calibrated: the radii, or fraction of the time-dependent similarity solution radius, at which the thermal conductivity and induction parameters are evaluated. This calibration is achieved by comparison with the results of a detailed time-dependent numerical flame simulation model which is a full solution of the multi-fluid conservation equations. The detailed model itself has been checked extensively with respect to its various chemical, diffusive transport, and hydrodynamic components.

The basic similarity solution is derived from the slow flow [6,7] approximation, characterized by (1) flow velocities which are small compared to the speed of sound, and (2) an essentially constant pressure field. The energy and velocity equations may then be written as

$$\frac{dP}{dt} \approx 0 = -\gamma P \underline{\nabla} \cdot \underline{v} + \underline{\nabla} \cdot \gamma N k_B \kappa \underline{\nabla} T + S(t) e^{-k^2(t) r^2}, \qquad (1)$$

from which we can derive an algebraic equation for $\underline{\nabla} \cdot \underline{v}$. Here P is the total pressure, $\underline{v}$ is the fluid velocity, T is the temperature, γ is the ratio of heat capacities C_p/C_v assumed here to be a constant and κ is a function of the mixture thermal conductivity, λ_m,

$$\kappa \equiv \frac{\gamma - 1}{\gamma N k_B} \lambda_m(T). \qquad (2)$$

The last term on the right hand side of Eq. (1) is the source term. Proper choice of S(t) ensures that a given amount of energy, E_o, is deposited in a certain volume, $\frac{4\pi}{3} R_o^3$, in a time, τ_o. The choice of this Gaussian profile allows us to obtain a "closed" form similarity solution. If the fluid velocity v is then expanded such that

$$v(r,t) \approx v_1(t) r \qquad (3)$$

and spherical symmetry is assumed, Eq. (1) may be solved analytically to obtain

$$T(r,t) = T_\infty e^{A(t) e^{-k^2(t) r^2}} \qquad (4)$$

and

$$\rho(r,t) = \rho_\infty \, e^{-A(t)e^{-k^2(t)r^2}}, \tag{5}$$

where T_∞ and ρ_∞ are the background temperature and density far from the heat source. Solutions for A(t) and k(t) may then be obtained by solving two coupled differential equations

$$\frac{dk}{dt} = - kv_1 - 2\kappa k^3 \tag{6}$$

$$\frac{dA}{dt} = \frac{S(t)}{\gamma P} - 6\kappa k^2 A. \tag{7}$$

Invoking energy conservation yields the expression for the velocity coefficient v_1, and is effectively the first calibration in the model:

$$v_1 = \frac{S}{3\gamma P_\infty} \frac{F'(0)-F'(A)}{F(A)} + 2\kappa k_B^2 \frac{AF'(A)-F(A)}{F(A)} \tag{8}$$

where the function F(A) is defined as

$$F(A) \equiv \int_0^\infty 4\pi x^2 [1-e^{-Ae^{-x^2}}]dx. \tag{9}$$

The model requires one further definition in order to predict ignition. A curve of chemical induction time as a function of temperature must be included in order to define the induction parameter,

$$I(t) = \int_0^t \frac{dt'}{\tau_c(T(r,t'))} \qquad (10)$$

Ignition "occurs" when $I(t) = 1$ in this model, which is an exact result in the limit of large heat source and constant temperature near the center of the heated region. A simple analytic expression for $\tau_c(T)$ depending on three constants has been derived and can be calibrated using as few as three distinct values of τ_c at different temperatures.

The chemical reaction scheme used in the detailed model was used to generate a curve for $\tau_c(T)$. The values of thermal conductivity used in the detailed model were used to generate a function κ. Then a series of comparisons were made, in which the detailed model was configured in spherical symmetry with a Gaussian energy deposition.

We show results for several test cases. In one, $R_o = 0.1$ cm and $\tau_o = 1 \times 10^{-4}$ sec. The simple model predicts that 3.3×10^4 ergs is the minimum ignition energy and these results agree well with the simulation (Figs. 7 and 8). Both models predict ignition at essentially the same time for a range of input energies. In the second example, $R_o = 0.025$ cm and $\tau_o = 1 \times 10^{-4}$ sec. The simplified model predicts a minimum ignition energy of $\sim 8 \times 10^2$ ergs. The full simulation does not show ignition, but predicts that some burning does occur and the flame is eventually quenched (Fig. 9). Thus in the regime for which both models agree, we have in fact tested them both. In the regime where they do not agree, we must then figure out what physics is missing from the similarity model. When this is done, we can, in effect, use the detailed model to

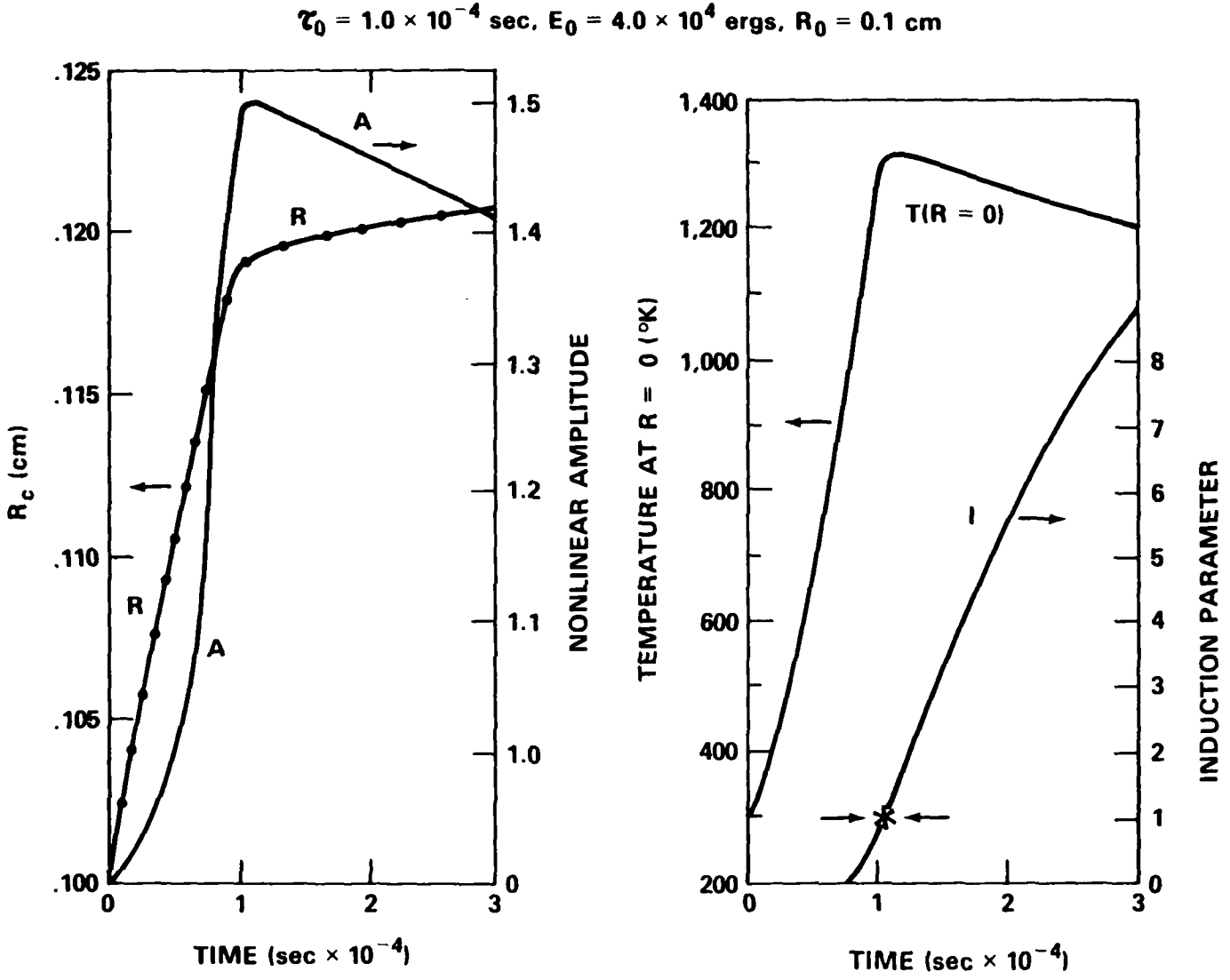


Fig. 7 - Calculated results from the similarity solution plotted as a function of time. Here R_c is the characteristic radius for energy deposition, A is the nonlinear amplitude of the temperature and density functions, T(R=0) is the central temperature and I is the induction parameter. The '*' indicates the predicted induction time.

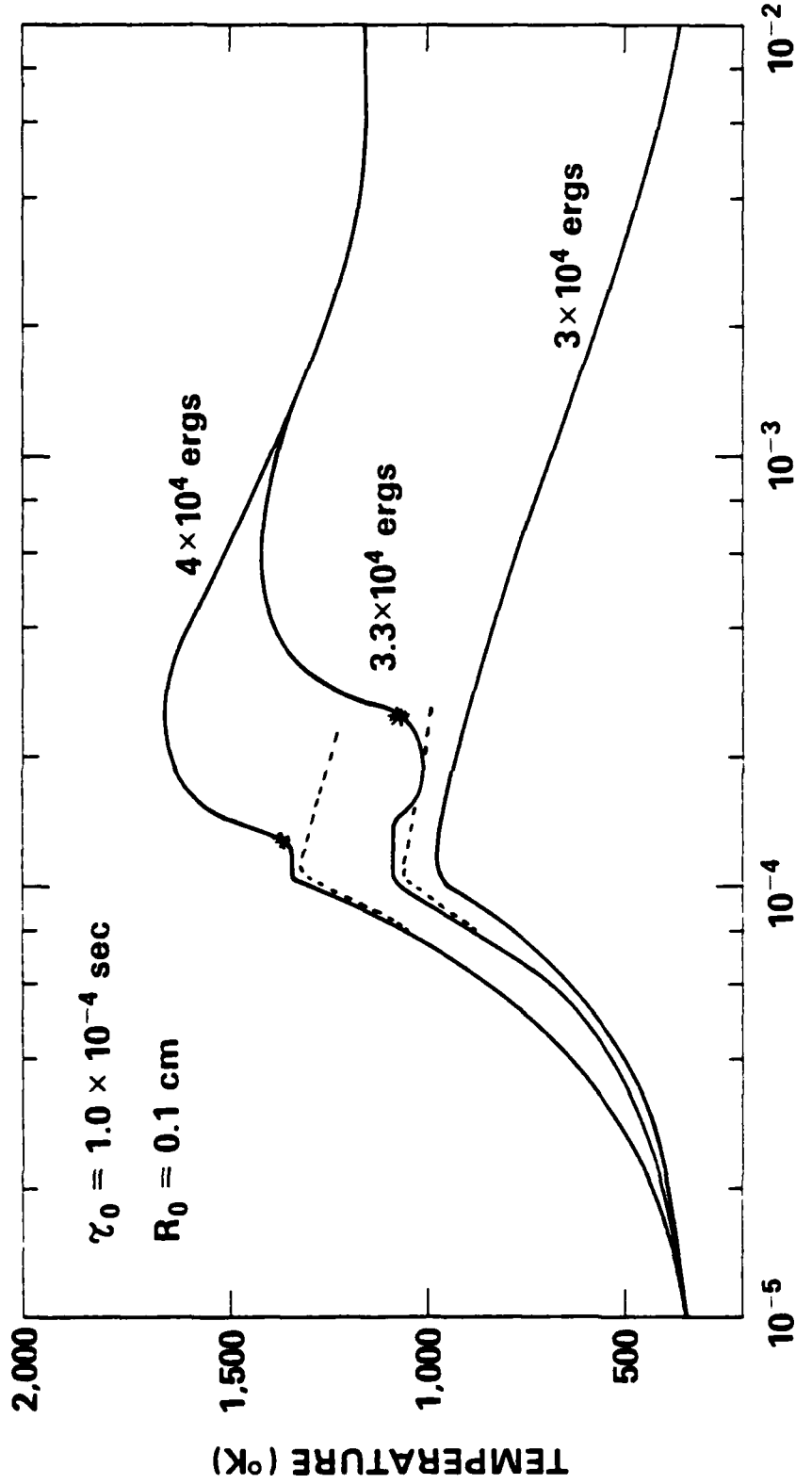


Fig. 8 - Comparisons of the similarity (dashed line) and detailed model (solid line) solutions for the central temperature as a function of time. The '*' marks the induction time predicted by the similarity solution.

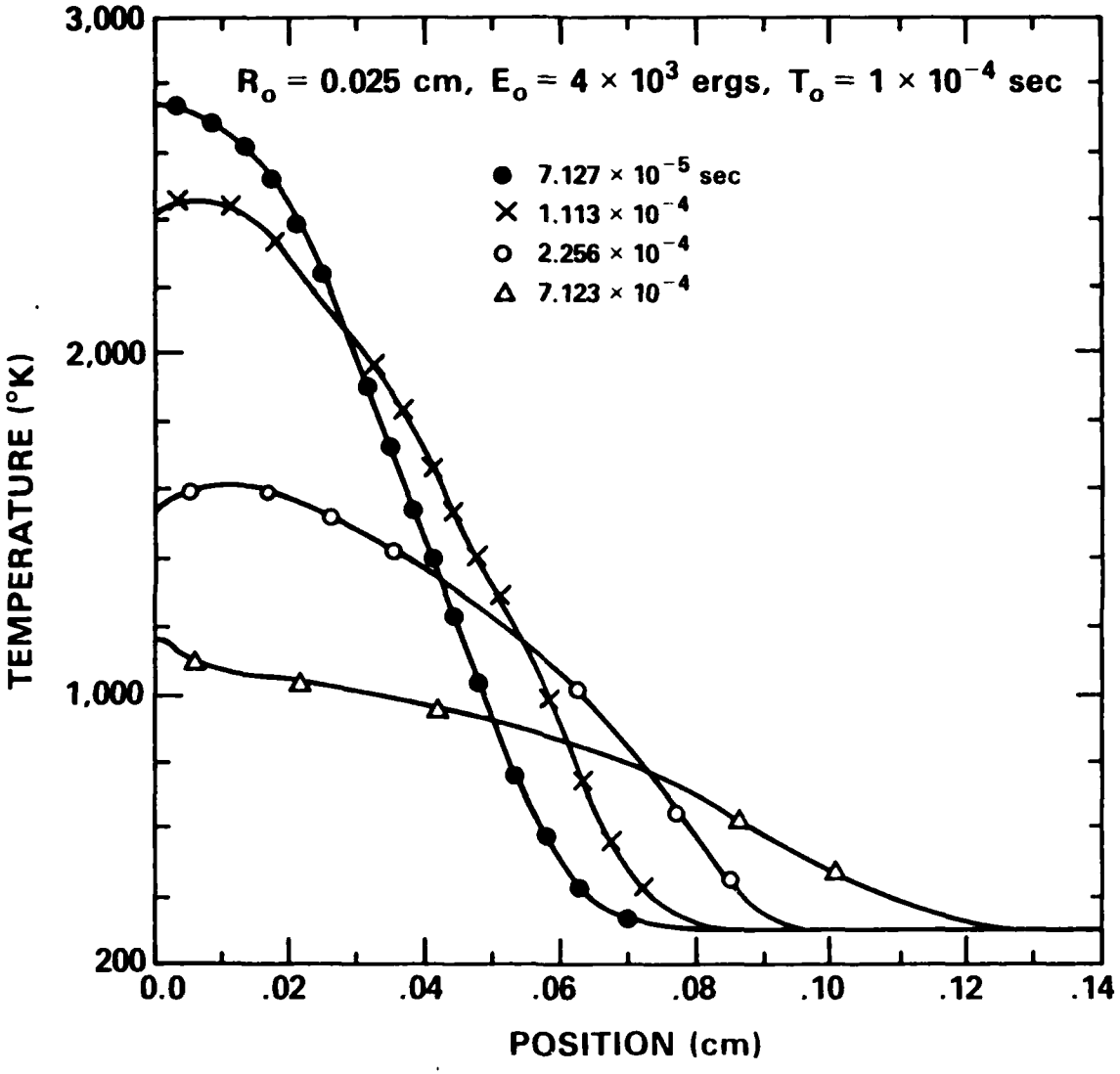


Fig. 9 - Temperature as a function of position at four times in the detailed flame model. The flame dies out even though the similarity solution indicates it should not.

build phenomenology into the similarity solution. The similarity solution has tested the full detailed model, and the full detailed model has shown us the limits of the similarity solution.

V. Testing the Model with Experiment

Although comparisons between analytic theory and model results can be used to extend our understanding of the controlling processes in a system with limited physical complexity, many systems may preclude any analytic formulation. Then experimental data provide the only means of checking the accuracy of the model. Below we show a case in which the results from an experiment were used to test a numerical model and the model results then suggested new directions for the experiments.

The determination of the effects of surface waves on submerged structures has many practical applications, particularly in an ocean environment. Due to the complexity of the problem, analytic results are limited to idealized flows and geometries. A major part of the complexity arises from the existence of the free surface itself. Not only does the free surface dominate the flow, but it may become multiply connected when sprays, wave-breaking or cavitation occur. There is usually no steady state, and a model for <u>transient</u> flow of the fluid over the obstacle must be used.

Here we describe the results of a model calculation of the wave-induced pressure forces on a submerged half-cylinder, and compare the results with experimental data. The implications of the comparisons for both the validity of the model and the experimental procedure will be

examined. Finally, the application of the model to other fluid flows and to combustion problems will be discussed.

Figure 10 illustrates the initial conditions for the numerical model. A half-cylinder of radius "a" is bmerged in a fluid whose undisturbed free surface stands at a height h = 2a over the bottom surface. A progressive wave with wavelength λ = 5a is incident on the cylinder from the left. The sides of the computational region are periodic: that is, the physical system being simulated is actually that of progressive waves over a series of half-cylinders. Periodic boundary conditions were chosen to avoid numerical damping and reflection at an outflow boundary. The calculation seeks to find the pressures at every point in the fluid as a function of time, and in particular the pressures and pressure gradient forces at points on the cylinder surface.

The numerical model is based on finite difference techniques for solving the equations for inviscid, incompressible fluid flow using a triangular grid which extends throughout the interior of the fluid [9]. The free surface and rigid boundary shapes are approximated by straight lines which extend between points on those surfaces and which define the edges of the computational grid. The governing equations are cast in a Lagrangian formalism so that points originally lying on a surface will remain there at all times during the calculation. Points interior to the fluid will follow Lagrangian pathlines as if they were experimental marker particles in a real fluid. The equations are differenced such that vorticity is conserved identically at all times and vertex pressures are chosen to be the values necessary to keep the local fluid

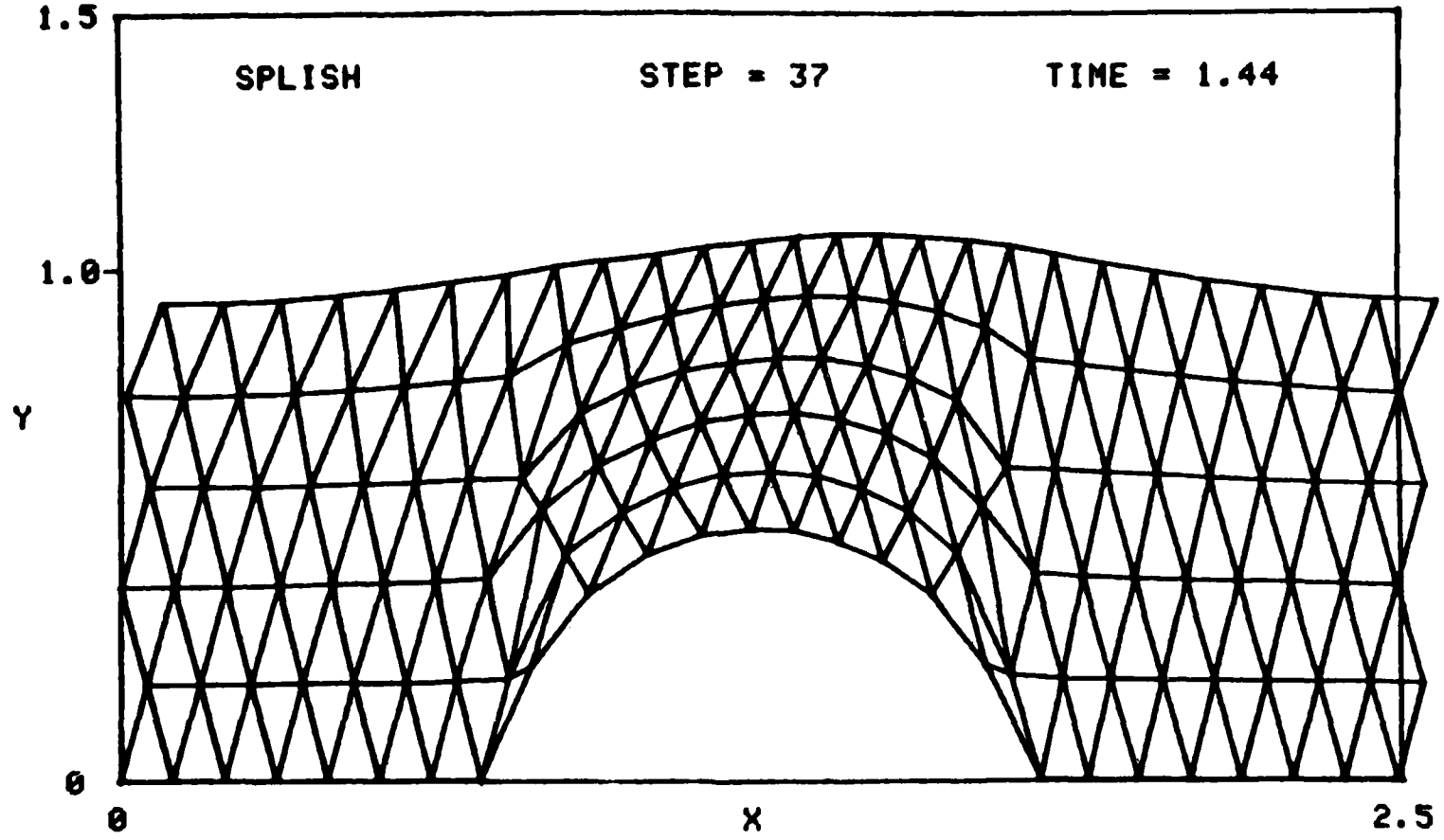


Fig. 10 - The triangular grid early in a calculation of wave flow over a half-cylinder. The first wave of a wave train has passed over the cylinder from the left.

volumes divergence-free. These new pressures are in turn used to advance the velocities and update the grid positions.

The physical behavior of the governing equations can be preserved in the approximate difference equations being solved numerically by using a triangular grid. A Lagrangian grid will distort in any non-trivial flow field, and as grid distortion becomes severe the calculation quickly loses accuracy. However, a triangular grid can be manipulated locally in several ways to extend realistic calculations of transient flows [9,10]. Each grid line represents a quadrilateral diagonal, and the opposite diagonal can be chosen whenever vertices move in the flow to positions which favor that connection. Such a reconnection involves just the four vertices describing the quadrilateral. No fluid moves relative to the quadrilateral, eliminating one form of numerical dissipation. Vertices may also be added or deleted to preserve the desired resolution by local algorithms which involve only those vertices in the vicinity of the grid anomaly. Major advantages of this technique are that the algorithms can be conservative, they permit a minimum of numerical dissipation and yet they require very little computer time since most of the grid remains unaltered.

Data for the experimental comparison was obtained through wave-tank experiments performed with a bottom-mounted half-cylinder so that pressure measurements could be compared directly to the numerical results [11]. The obstacle was placed one-third of the tank length from a mechanical wavemaker and at the other end of the channel a sloping porous beach absorbed 95% or more of the incident wave energy.

Results of the experiment and of the numerical simulation are shown in Figure 11, together with the results of linear theory. The magnitude of the pressure fluctuations as measured by the experiment at different points on the cylinder ($\theta = 0°$ at the top of the cylinder) are compared with the predictions of the model. As shown in Figure 11, the comparison is quite good. Figure 12 compares the calculated and measured instantaneous pressure distribution around the cylinder for the situation in which the crest of the progressive wave is near the left side of the half-cylinder. Again the comparisons look good, but now some differences become evident.

It was found that to within experimental error, all of the observed discrepancies could be explained by two factors. The first factor is that the model did not exactly describe the physical situation in the experiment: the wave tank had a single cylinder whereas the calculation is for a series of cylinders. The second factor was the surprising result that the roughly 5% reflected wave from the wave tank significantly affected the experimental results due to modifications in the dynamic pressure fluctuations. In this instance a detailed examination of the model and experimental results has indicated that an experimental effect thought to be small could in fact cause noticeable deviations in the data measured.

The application of this numerical technique to reactive flow is relatively straightforward. Although the example presented above is for homogeneous flows, the extension to include interfaces involves no basic changes to the underlying gridding scheme, but only the provision

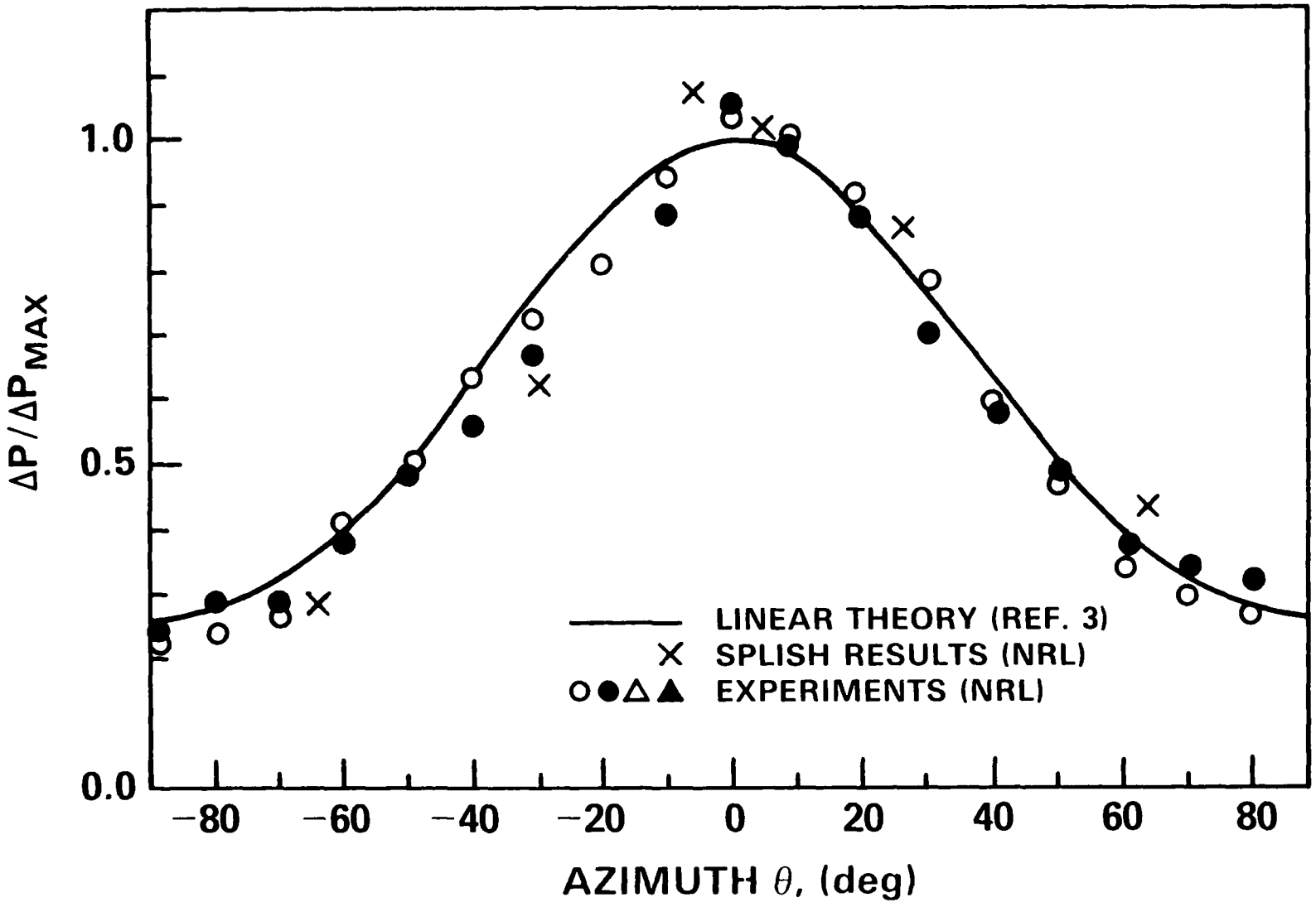
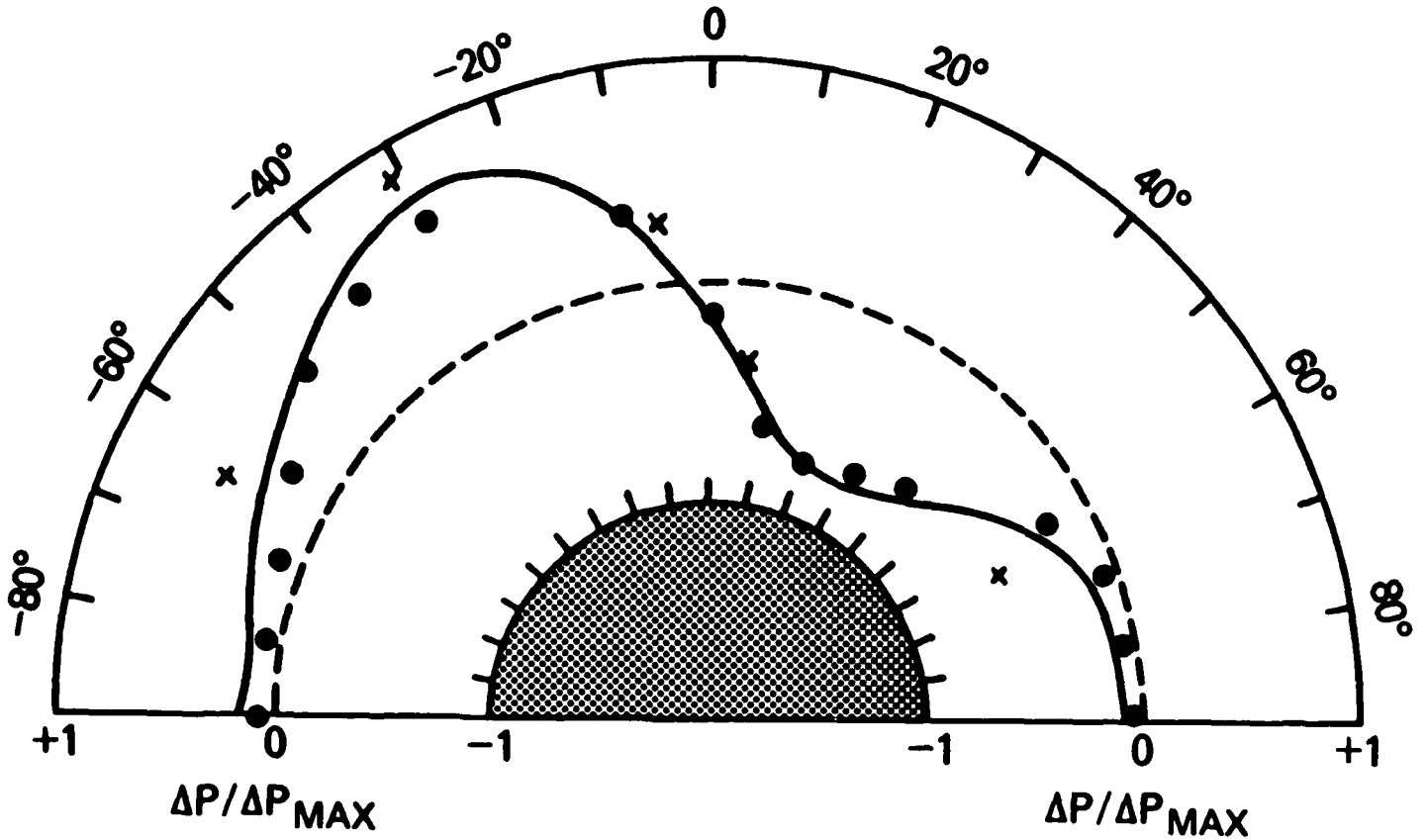


Fig. 11 - A comparison of numerical results with experiment and with linear theory for the magnitude of pressure variations over a half-cylinder due to a progressive wave with ka = w.5, kh = 5.



LINEAR THEORY (REF. 3)
× SPLISH RESULTS (NRL)
● EXPERIMENTS (NRL)

Fig. 12 - A comparison of numerical results with theory and experiment for instantaneous pressure distributions on a half-cylinder (ka = 2.5, kh = 5), with the wave crest just to the left of the cylinder

that no interface sides are allowed to be reconnected. Instead local gridding anomalies at the interfaces are resolved by adding or subtracting vertices at the interface and reconnecting grid lines leading to those vertices. That this solution is viable is most easily shown by Fig. 13 which shows stages in the collapse of a Rayleigh-Taylor unstable fluid layer calculated with the same model. Here the calculation can continue even though the originally simply-connected lighter fluid performs a transition to a multiply connected fluid which includes "bubbles" which have been entrained by the heavier fluid. Of course, for reactive flow calculations a new model would have to be constructed based on these techniques which used instead the equations governing compressible fluids and which contained the added chemical and thermal equations besides.

VI. Conclusion

Deatiled modelling of laminar reactive flows, even in fairly complicated geometries, is certainly well within our current capabilities. In this paper we have shown several ways in which these techniques may be used. As the physical complexity we wish to model increases, our footing becomes less sure and more phenomenology must be added. For example, we might have to add evaporation laws at liquid-gas interfaces or less well-known chemical reaction rates in complex hydrocarbon fuels.

Perhaps the biggest problem facing combustion modelling now is turbulence: there are no excellent or even good methods of including such effects in our calculations. At best we have a number of phenomenological models with limited ranges of validity and which imply a steady state.

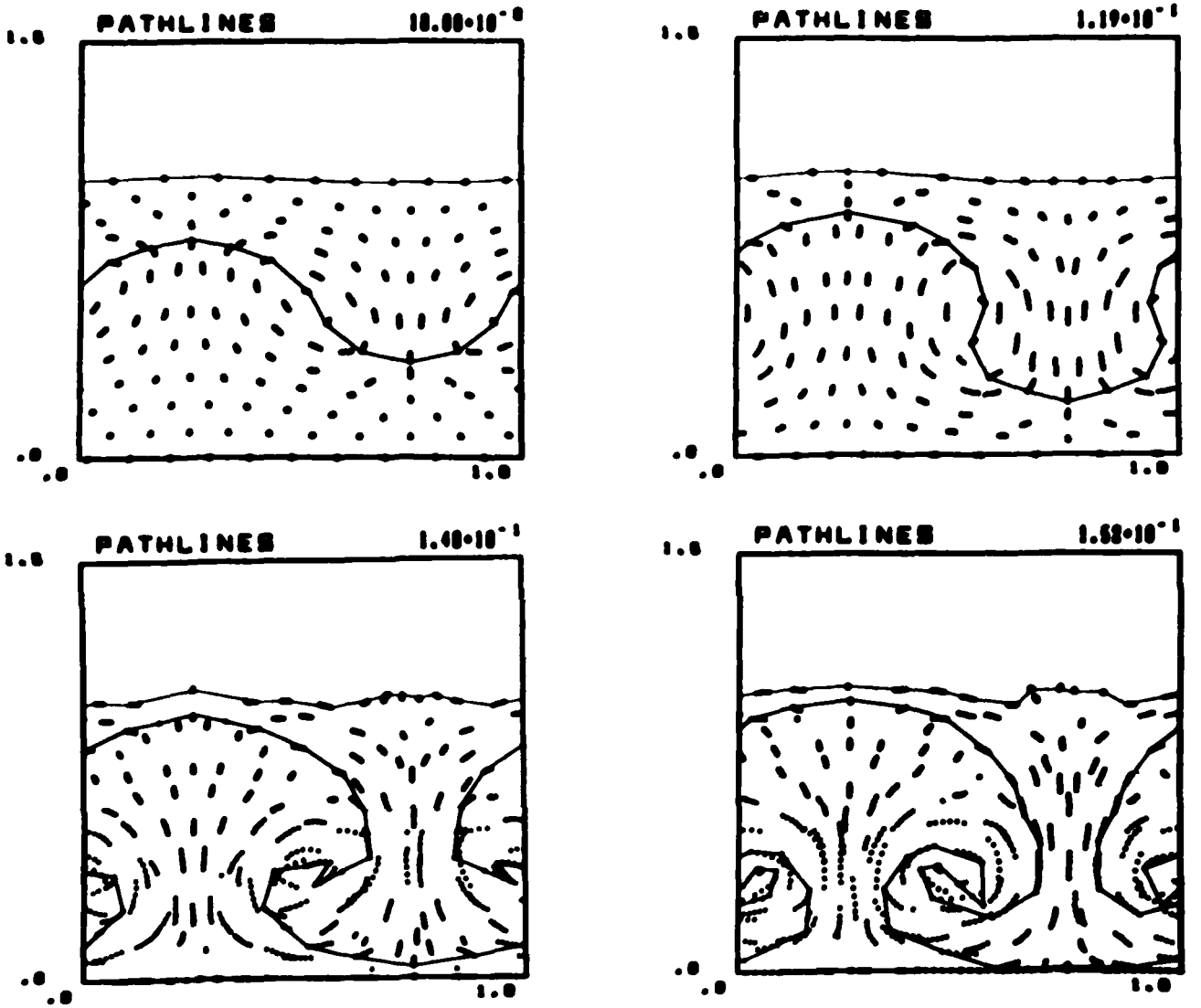


Fig. 13 - Lagrangian pathlines at various stages of a Rayleigh-Taylor collapse for the case of two inviscid, incompressible fluids having a density ratio of 2:1. A free surface is present above the dense fluid and the interface between the fluids is indicated for each stage. The simulation shows how later evolution of the fluid flow is dominated by the strength and dynamics of the vortex pair created during the early stages of collapse.

We believe that devising a way to handle this difficult problem of strongly coupled multiple time and space scales is the challenge we currently face.

Acknowledgments

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